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3D Simulation of Ammonia Combustion in a Lean Premixed Swirl Burner

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Abstract

To date, a number of mechanical, electrical, thermal, and chemical approaches have been developed for storing electrical energy for utility-scale services. The only sufficiently flexible mechanism allowing large quantities of energy to be stored over long time periods is chemical energy storage in the form of carbon or hydrogen. One chemical considered for hydrogen carriage that can potentially be employed for storage is ammonia. Ammonia can substitute pure hydrogen for storage and be employed for power generation at large industrial scale if the molecule is efficiently burned through mature equipment such as gas turbines, thus providing not only a carbon free fuel, but also a chemical capable of being stored at low energy requirements. Thus, progress on the use of ammonia in gas turbines is a main priority for groups working on the area. Studies need to be conducted in experimental rigs with strong CFD analyses for further industrial implementation. In this paper, modelling of ammonia combustion in a generic gas turbine combustor is explored in order to provide an effective tool for future application. Large Eddy Simulation approach was used to develop a model for ammonia/hydrogen combustion in gas turbine combustors. To capture more details of the turbulent reacting flow, a detailed chemical mechanism was selected for a deep insight. A Partially Stirred Reactor framework was utilized to deal with the turbulence/chemistry interaction. The developed model was then applied to the simulation of lean premixed ammonia/hydrogen flames in a generic swirl burner. A preliminary validation for the model is performed by correlation of NOx emission with experimental data. Results show the model can provide detailed information of flow field, flame structure, emissions, etc. It can be used to optimize the procedure of utilizing ammonia as a fuel in future equipment design.

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1 Introduction

Environmental problems caused by excessive use of fossil fuels are amongst the top governmental, research and industrial agendas. Under this situation, requirements for new environmental friendly fuel systems to replace fossil fuel technologies are key. Ammonia, as a carbon-free fuel, has the potential to be the novel fuel for future energy systems. Ammonia has high hydrogen contents (17%) and yields only water and nitrogen as combustion products when completely burned. It is also a major product in chemical industry, so there are already many infrastructures and much experience regarding its handling. Besides, ammonia is safer than hydrogen and various other fuels, especially during transportation, storage and distribution which are difficult problems for hydrogen.

Currently, there are several examples and studies trying to utilize ammonia for power systems especially in internal combustion engines [1]. However, power obtained from such units is relatively modest on utility scales, typically in the range of 0.1 – 1 MW only. Thus similarly responsive but more powerful energy release devices will be required to meet the demands of power grids. As a result, considering the big pressure to reduce carbon dioxide emission and the ever-rising price of conventional fuels, using ammonia in gas turbines for power generation is quite attractive.

Although research has been undertaken for operational flame limits, chemical models, flame speed and internal combustion engines, gas turbines have played a minor role using this fuel [2]. Groups that have shown some development on the understanding of these systems are limited [3, 4]. Results showed series of challenges when using this fuel [5]. Swirl stabilised combustion of ammonia with other molecules has briefly been analysed by Meyer et al.[6] in a 40kW burner, with nozzles, swirl stabilisers and a self-sustained heat exchanger. Stabilisation was achieved using different swirlers with different concentrations of ammonia, hydrogen and methane. Experiments demonstrated a reduction in NOx emissions through flue gas recirculation. The Fukishima Renewable Energy Institute (FREA), has also developed new platforms to burn liquid ammonia from wind and solar energy combined with kerosene in a 50 kW micro-gas turbine [7]. It has been demonstrated that the equipment can be run using ammonia-kerosene blends at different concentrations. However, ammonia/hydrogen blends have seldom been documented for power generation in gas turbines [8]. Since the use of this blend will not produce CO2 emissions, its adequate understanding will provide the foundations to progress into more advanced blends comprised by hydrogen and ammonia.

To explore the feasibility of using these ammonia blends in a gas turbine, it is essential to study their combustion characteristics. Part of the study needs to be developed through new simulation tools in order to reduce implementation time. Combustion in gas turbine is a complex phenomenon which is combination of turbulence, reaction, heat transfer, etc. In conjunction with ammonia as a relatively new fuel, the simulation process faces many difficulties such as the need of high resolution meshes for complex geometries, chemical kinetic mechanism for ammonia combustion, description of turbulence/reaction interactions, etc. Among them, detailed chemical kinetic mechanisms need to be carefully considered to achieve good CFD analyses for appropriate ammonia combustion simulations, representative of experimental tests and applicable to industrial designs. Thus, there is a need to reduce the detailed ammonia combustion mechanisms and test them under conditions of a typical gas turbine combustor. With seldom study on the field, it is clear that there is a great opportunity in the area to develop new mechanisms, CFD simulations, experimental setups and industrial designs.

Therefore, it is clear that there is a considerable knowledge gap for the development of ammonia fueled based power systems and a growing interest in the field from industry and academia. Thus, this paper presents numerical and experimental results for a representative, land-based gas turbine combustor running on ammonia-hydrogen blends. Studies were performed to observe the progression of the flame under lean premixed conditions with the aim of finding data relevant for the development of new ammonia combustors for large-scale power generation. LES framework combined with detailed chemistry has been employed for modelling the turbulent combustion of ammonia in a generic gas turbine combustor, with correlation with experiments performed in a parallel project.

2 Numerical Modelling

For the 3D numerical simulation, the approaches are mainly Reynolds-Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). Between RANS and DNS sits LES, which is increasingly becoming a reliable tool for gas turbines. Since chemical reactions in the combustion occur at such small scales, the advantage of LES is considered promising in this area [9]. Thus, it was decided to use LES in this study.

2.1 Turbulence Model

The implementation of Large Eddy Simulation for turbulent combustion firstly needs to spatially filter the conservation equations so as to separate eddies of large scales from small scales. The well-established Favre-filtered conservation equations (mass, momentum, energy and species) are employed [9].

The filter and average process inevitably leaves the sub-grid eddies unclosed, so sub-grid scale (SGS) models are needed to solve those terms. The SGS stress tensor is usually addressed using various models. One of the most commonly used is the Smagorinsky model [9] which is utilised for SGS closure in this study.

2.2 Chemical Kinetic Model

Chemical kinetic modelling is fundamentally important through these simulations. Therefore, a detailed chemical mechanism was required. It is reported that Konnov's mechanism [10] agrees well with experiments for the prediction of NO which is the main emission obtained from ammonia combustion in gas turbine. However, Konnov's mechanism contains more than 1000 steps and 106 species, making it prohibitive for the resolution of 3D LES combustion simulation in a representative gas turbine combustor in terms of computational time in our facilities. Thus, considering the size of the mechanism, a reduced mechanism was used in the 3D simulation. As it will be seen later, the mechanism has good agreement with experiments at those fuel lean conditions that were numerically analysed.

2.3 Combustion Model

To deal with the chemical source term in the conservation equation, a SGS combustion model was required. The modelling approach employed in this study is the Partially Stirred Reactor (PaSR) which can account for the turbulence/chemistry interaction. The PaSR concept proposed by Karlsson[11] has proved effective in turbulent combustion simulations. Besides, since it can offer complex chemistry treatment, it is suitable for the simulation of combustion in this study under realistic premixing applications.

Under the PaSR framework, a computational cell is split into the reacting and non-reacting zones. In reacting zones, each specie is assumed to be homogeneously mixed with each other being under perfectly stirred reactor (PSR) conditions. Meanwhile, in the non-reacting zones it is assumed that no reaction occurs. Thus, the key issue to apply the PaSR concept is to figure out the mass fraction of the reacting zones.

2.4 Numerical Setup

The simulation in this study was implemented by using a fully compressible solver for combustion under the OpenFOAM platform [12]. The governing equations were solved implicitly using the finite volume method in which a 2^{nd} order scheme was employed for time stepping and spatial discretisation. The maximum courant number was set to 0.5 and physical time step was set to $5e^{-6}$ s.

To use a high quality mesh, a structured system containing about 0.8 million cells was generated for the simulation of the can combustor, Fig. 1. This system is representative of an experimental system developed at the Gas Turbine Research Centre (GTRC), Cardiff University, Fig. 1. Further details of this experimental rig can be found in [13]. The mesh was refined in the middle section to better capture turbulence and reactions across the flame, Fig. 2. Specific boundary conditions for this study are listed in Table 1. Numerical results were compared and correlated to experimental data obtained in previous campaigns through a program dedicated to develop gas turbine combustors using ammonia blends for power generation.

Fig. 1. Overview of burner configuration and grid configuration

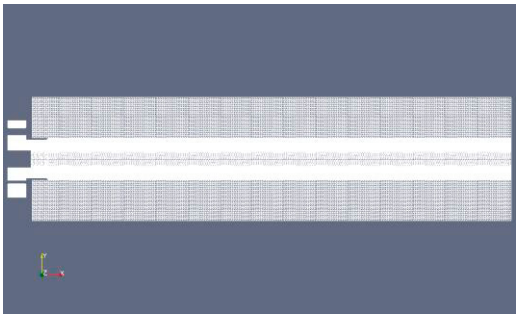

Fig. 2. Mesh of the combustor

Table 1. Boundary conditions of combustor model

Operating pressure		1atm
Oxidiser (mol%)	O2	21%
	N2	79%
Fuel (mol%)	NH3	50%
	H2	50%
Power		30kW
Ambient Temperature		300K

3 Results and Discussion

3.1 Model validation

Fig. 3 compares the NO emission obtained by LES simulation with experimental results [13]. The results are obtained after running the model for 60,000 time steps (0.3 s), when the fluid field does not show remarkable variation. It can be seen that the model has predicted the trend of NO emission varied with equivalence ratio generally. Although more detailed validation work is still expected, confidence on the results allowed further comparisons.

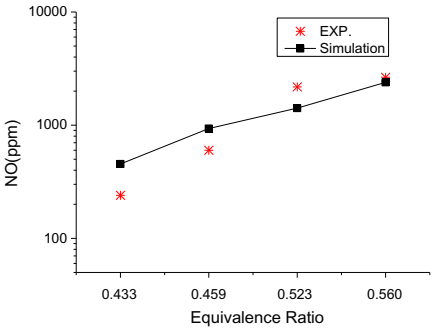

Fig. 3. NO emission results compared to simulation.

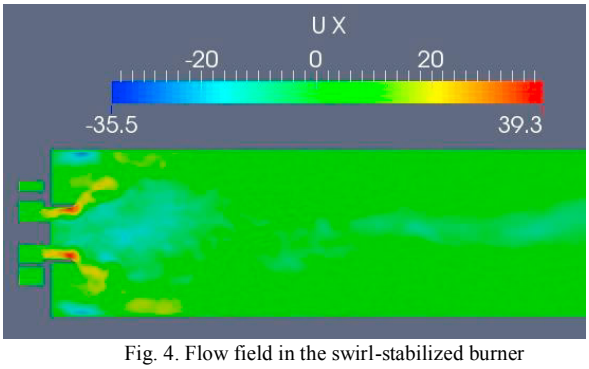

Fig. 4. Flow field in the swirl-stabilized burner

3.2 Ammonia/hydrogen flame in swirl burner

Fig. 4 shows flame behaviour illustrated by flow field associated with swirl burner configurations at an equivalence ratio of 0.56. As shown, two kinds of recirculation zones are generated at the flow downstream of the inlet. A coherent central recirculation zone (CRZ) has been formed stabilising the flame. This CRZ degrades into a long, low velocity tail as observed experimentally [13]. Thus, a fully developed swirling flow acted on the combustion process. Also, there are typically corner recirculation zones as shown at the corner of the quartz confinement tube intersecting the horizontal inlet plate.

The numerical simulation results also provide an overview of progression of several species, Figs. 5 to 7. It is clear that considerable amounts of OH radicals are produced and consumed close to the dump plane ~0.5D from the nozzle, Fig. 5. The outer edge shape of high OH regions is irregular corresponding to the velocity distribution in Fig.

4. As expected, these radicals keep reducing their concentration as they move downstream. Their consumption happens through various reactions that increase temperature, Fig. 6.

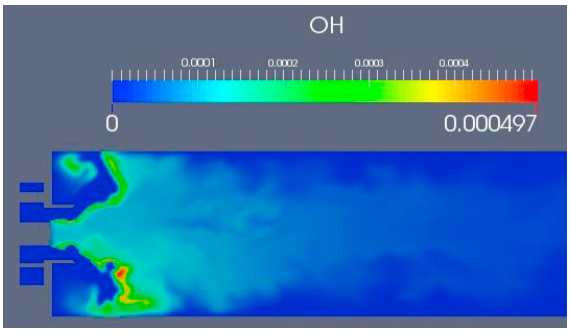

Fig. 5. OH distribution across the burner (mass fraction).

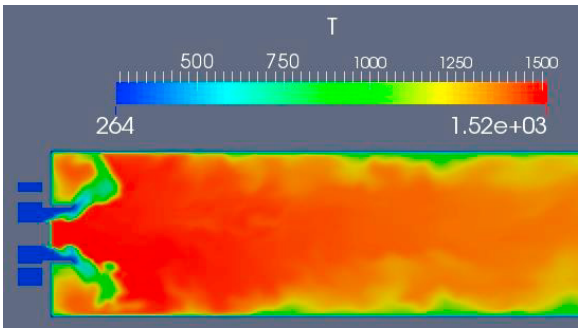

Fig. 6. Temperature distribution across the burner. [K]

Considerable NO production takes place across the boundaries of the flame, Fig. 7. This expected behaviour is a consequence of the high temperatures of combustion and recombination of species, mainly through the chemical paths NH2+OH→NH+OH→NO and NH2+O→HNO+OH→NO. High NO concentration produced at the nozzle is then diluted downstream the flame zone.

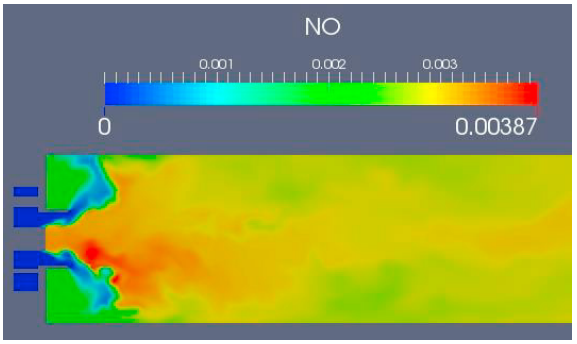

Fig. 7. NO distribution across the burner (mass fraction).

4 Conclusions

This is the first 3D simulation work to study ammonia/hydrogen combustion in a generic swirl burner. The open source solver OpenFOAM, was used to characterise the lean premixed turbulent flame in a laboratory-scale gas turbine swirl burner, which has been experimentally tested previously with ammonia/hydrogen fuel blends.

Fundamental chemical kinetic mechanism knowledge was employed for the simulation work. Because of the extremely high computational cost needed to run detailed chemical mechanisms, a reduced mechanism was implemented in this LES modelling study.

Preliminary validation of the model was performed by correlation to predict NOx with previous experimental trials. Although it was observed that the trend of experimentally measurable species was in good correlation, some other species and flow field data are need for further comparisons.

Flame structure was then studied using the model developed. Information of flow field, temperature, species such as OH and NO were obtained effectively. Results recognised that premixed flames can be stabilised in the swirl burner but NOx emission is still high. Therefore, new stratified injection techniques need to be developed to reduce these disadvantages and employ radicals and product species more efficiently through the combustion process.

This study confirms that LES modelling can be used to study lean premixed combustion of ammonia/hydrogen numerically. The results will be used in an ongoing project to optimize the procedure of utilizing ammonia in gas turbine combustors.

5 Acknowledges

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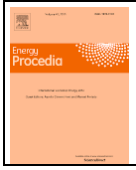
References

[1] F.R. Westlye, A. Ivarsson, J. Schramm, Experimental investigation of nitrogen based emissions from an ammonia fueled SI-engine, Fuel, 111 (2013) 239-247.
[2] H. Xiao, A. Valera-Medina, R. Marsh, P.J. Bowen, Numerical study assessing various ammonia/methane reaction models for use under gas turbine conditions, Fuel, 196 (2017) 344-351.
[3] H. Xiao, M. Howard, A. Valera-Medina, S. Dooley, P.J. Bowen, Study on Reduced Chemical Mechanisms of Ammonia/Methane Combustion under Gas Turbine Conditions, Energy & Fuels, 30 (2016) 8701-8710.
[4] C. Zamfirescu, I. Dincer, Ammonia as a green fuel and hydrogen source for vehicular applications, Fuel Processing Technology, 90 (2009) 729-737.
[5] J. Ganley, Increasing the Combustibility of NH3 Fuel. https://nh3fuelassociation.org/events-conferences/2010-nh3-fuel-conference/, in: 2010 Annual NH3 Fuel Conference 2010.
[6] T. Meyer, P. Kumar, M. Li, Ammonia combustion with near-zero pollutant emissions. NH3 Fuel Association, January 2011. [Online]. Available: https://nh3fuel.files.wordpress.com/2013/01/2011-meyer.pdf. [Accessed 12 November 2016]. in, 2011.
[7] N. Iki, O. Kurata, T. Matsunuma, T. Inoue, M. Suzuki, T. Tsujimura, H. Furutani, Micro Gas Turbine Firing Kerosene and Ammonia, in: ASME Turbo Expo 2015: Turbine Technical Conference and Exposition, American Society of Mechanical Engineers, 2015, pp. V008T023A023-V008T023A023.
[8] H. Xiao, A. Valera-Medina, Chemical Kinetic Mechanism Study on Premixed Combustion of Ammonia/Hydrogen Fuels for Gas Turbine Use, Journal of Engineering for Gas Turbines and Power, 139 (2017) 081504.
[9] F. di Mare, W.P. Jones, K.R. Menzies, Large eddy simulation of a model gas turbine combustor, Combustion and Flame, 137 (2004) 278-294.
[10] A.A. Konnov, Implementation of the NCN pathway of prompt-NO formation in the detailed reaction mechanism, Combustion and Flame, 156 (2009) 2093-2105.
[11] N.N. Golovitchev V., Jarnicki R., 3-D diesel spray simulations using a new detailed chemistry turbulent combustion model, SAE Technical Paper, No. 2000-01-1891 (2000).
[12] F. Tao, V.I. Golovitchev, J. Chomiak, A phenomenological model for the prediction of soot formation in diesel spray combustion, Combustion and Flame, 136 (2004) 270-282.
[13] A. Valera-Medina, S. Morris, J. Runyon, D.G. Pugh, R. Marsh, P. Beasley, T. Hughes, Ammonia, Methane and Hydrogen for Gas Turbines, Energy Procedia, 75 (2015) 118-123.



Biography

Mr. Xiao is a Ph.D. candidate at Cardiff University. He works on topics about combustion of green fuels in gas turbine.